

5/09/05

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PASSWORD:

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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADO
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/IMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced
NEWS	16	APR 18	New CAS Information Use Policies available online
NEWS	17	APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	18	APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 17:40:59 ON 09 MAY 2005

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 17:41:07 ON 09 MAY 2005

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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 8 MAY 2005 HIGHEST RN 850006-33-6

DICTIONARY FILE UPDATES: 8 MAY 2005 HIGHEST RN 850006-33-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:

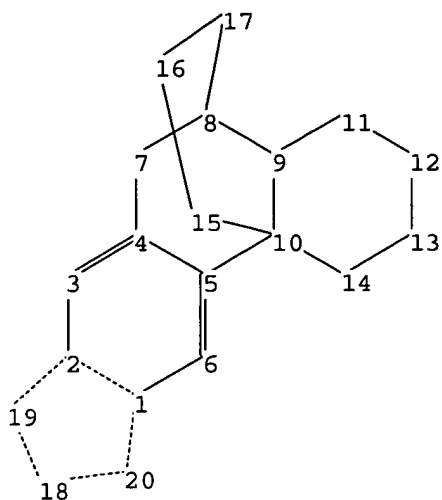
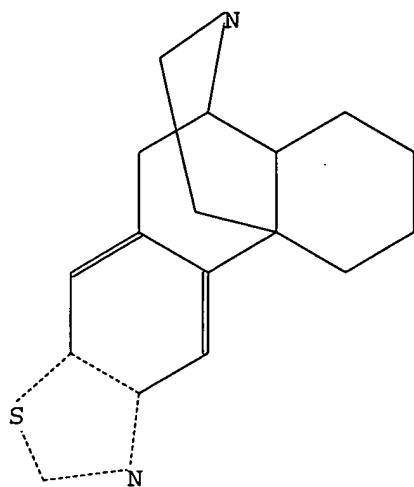
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10716100.str

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ring nodes :
1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20
ring bonds :
1-2 1-6 1-20 2-3 2-19 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-17 9-10 9-11
10-14 10-15 11-12 12-13 13-14 15-16 16-17 18-19 18-20
exact/norm bonds :
1-2 1-6 1-20 2-3 2-19 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-17 9-10 9-11
10-14 10-15 11-12 12-13 13-14 15-16 16-17 18-19 18-20
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom
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L1 STRUCTURE UPLOADED

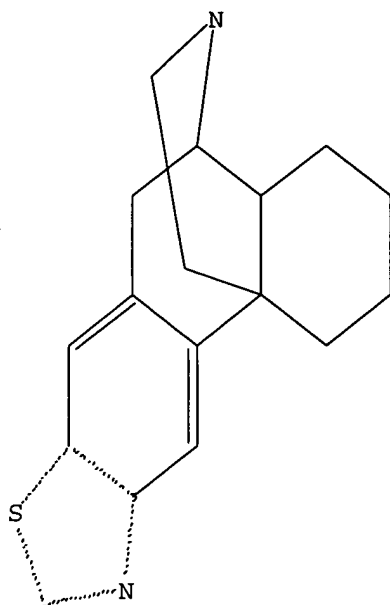
=> d l1

L1 HAS NO ANSWERS

L1 STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 17:41:27 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 56 TO 504  
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 17:41:33 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 261 TO ITERATE

100.0% PROCESSED 261 ITERATIONS 36 ANSWERS  
SEARCH TIME: 00.00.01

L3 36 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 17:41:36 ON 09 MAY 2005  
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FILE COVERS 1907 - 9 May 2005 VOL 142 ISS 20

FILE LAST UPDATED: 8 May 2005 (20050508/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

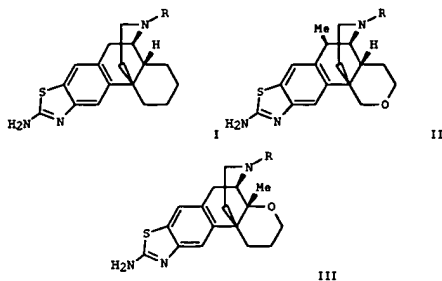
=> s l3

L4                    3 L3

=> d abs hitstr 1-3

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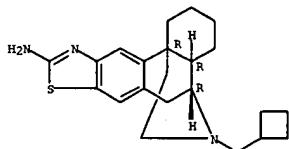
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
G1



AB Various types (i.e. I, II, and III (R = H, C1-7 alkyl, C2-7 alkenyl, C2-7 alkynyl, C2-6 heterocyclyl, C6-12 aryl, C7-14 alkaryl, C3-10 alkheterocyclyl, and C1-7 heteroalkyl)) of kappa and mu opioids were prepared for the treatment of pain or a dopamine dysregulation disease, such as schizophrenia, attention deficit hyperactivity disorder (ADHD), attention deficit hyperactivity disorder (ADD), Parkinson's disease, hyperprolactinemia, depression, and addiction. Thus, levorphanol was treated with N-Ph bis(trifluoromethanesulfonimide) and triethylamine to yield the triflate which was reduced using Pd/C (10%) and ammonium formate to give N-Me morphinan. N-Me morphinan was nitrated using HNO<sub>3</sub>/H<sub>2</sub>SO<sub>4</sub> in nitromethanol to give 2-nitro-N-methylmorphinan which was reduced to the amine using Pd/C (10%) and ammonium formate in methanol. Treatment of them amine with potassium thiocyanate and bromine in acetic acid gave the aminothiazole I (R = Me) which has a Ki of 130 nM for the  $\mu$  receptor and a Ki of 29 nM for the kappa opioid receptor.

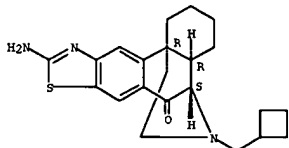
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696592-94-6P 696592-96-8P 696592-98-0P  
696593-00-7P 696593-02-9P 696593-04-1P  
696593-06-3P 696593-08-5P 696593-10-9P  
696593-12-1P 696593-14-3P 696593-16-5P  
696597-14-5P 696597-21-4P 696597-24-7P  
696597-27-0P 696597-30-1P 696597-33-9P  
696597-36-1P 696597-40-7P 696597-46-3P  
696597-51-0P 696597-54-3P 696597-58-7P  
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L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



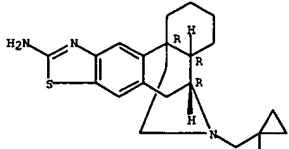
RN 682806-56-0 CAPLUS  
CN 6H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-(cyclobutylmethyl)-1,2,3,4,4a,5,6-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696592-90-2 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-[(1-methylcyclopropyl)methyl]-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

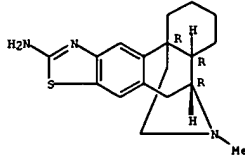


RN 696592-92-4 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-(3-fluoropropyl)-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

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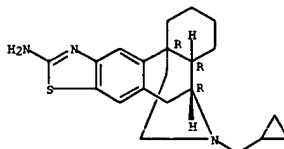
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of opioid receptor binders for the treatment of pain or dopamine dysregulation diseases)  
RN 609809-84-9 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-methyl-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 682806-53-7 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 14-(cyclopropylmethyl)-2,3,4,4a,5,6-hexahydro-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

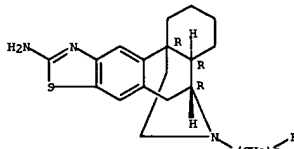


RN 682806-55-9 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 14-(cyclobutylmethyl)-2,3,4,4a,5,6-hexahydro-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

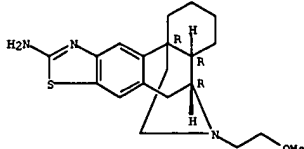
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.



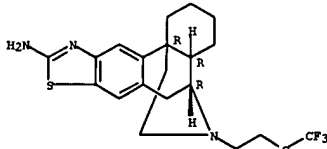
RN 696592-94-6 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-(2-methoxyethyl)-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696592-96-8 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-[2-(trifluoromethoxy)ethyl]-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

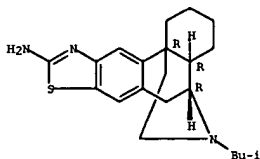


RN 696592-98-0 CAPLUS  
CN 1H-5,11b-(Iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-(2-methylpropyl)-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

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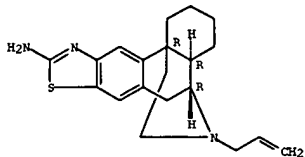
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
INDEX NAME]

Absolute stereochemistry.



RN 696593-00-7 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
2,3,4,4a,5,6-hexahydro-14-(2-propenyl)-, (4aR,5R,11bR)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.

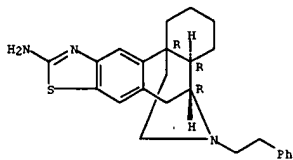


RN 696593-02-9 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
2,3,4,4a,5,6-hexahydro-14-[(2E)-3-iodo-2-propenyl]-, (4aR,5R,11bR)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

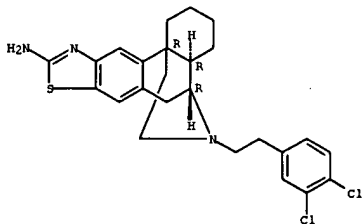
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
2,3,4,4a,5,6-hexahydro-14-(2-phenylethyl)-, (4aR,5R,11bR)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



RN 696593-10-9 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
14-[(2-(3,4-dichlorophenyl)ethyl)-2,3,4,4a,5,6-hexahydro-], (4aR,5R,11bR)-  
(9CI) (CA INDEX NAME)

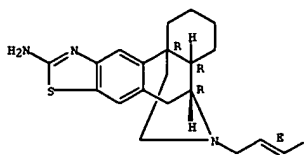
Absolute stereochemistry.



RN 696593-12-1 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
14-[(3-furanylmethyl)-2,3,4,4a,5,6-hexahydro-], (4aR,5R,11bR)- (9CI) (CA  
INDEX NAME)

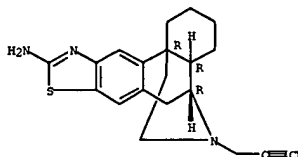
Absolute stereochemistry.

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



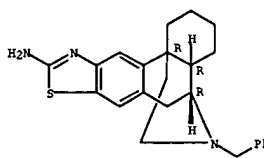
RN 696593-04-1 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
2,3,4,4a,5,6-hexahydro-14-(2-propynyl)-, (4aR,5R,11bR)- (9CI) (CA INDEX  
NAME)

Absolute stereochemistry.



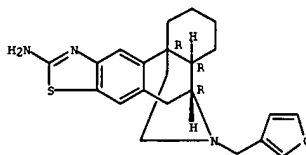
RN 696593-06-3 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
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NAME)

Absolute stereochemistry.



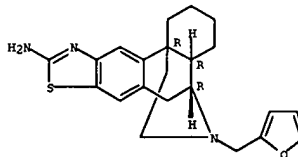
RN 696593-08-5 CAPLUS

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



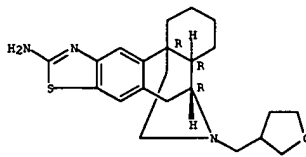
RN 696593-14-3 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
14-[(2-furanylmethyl)-2,3,4,4a,5,6-hexahydro-], (4aR,5R,11bR)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



RN 696593-16-5 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine,  
2,3,4,4a,5,6-hexahydro-14-[(tetrahydro-3-furanyl)methyl]-, (4aR,5R,11bR)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



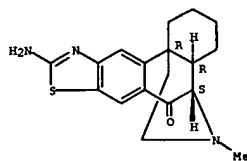
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CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5,6-hexahydro-14-methyl-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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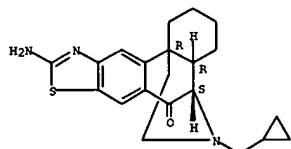
5/09/05

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



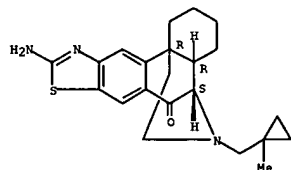
RN 696597-21-4 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-(cyclopropylmethyl)-1,2,3,4,4a,5-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

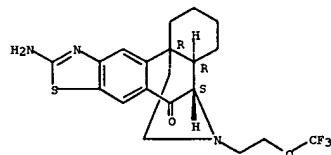


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CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-[[1-methylcyclopropyl)methyl]-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

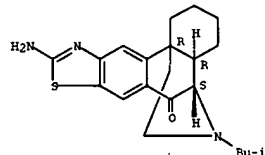


L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



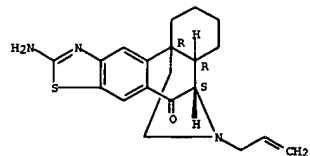
RN 696597-36-1 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(2-methylpropyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696597-40-7 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(2-propenyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696597-46-3 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-[(2E)-3-iodo-2-propenyl]-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

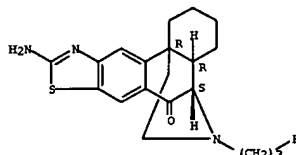
Absolute stereochemistry.  
Double bond geometry as shown.

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L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

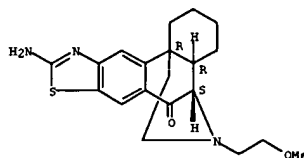
RN 696597-27-0 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-(3-fluoropropyl)-1,2,3,4,4a,5-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696597-30-5 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(2-methoxyethyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

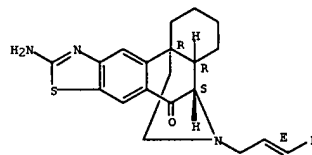
Absolute stereochemistry.



RN 696597-33-8 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-[2-(trifluoromethoxy)ethyl]-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

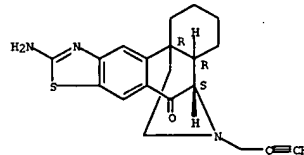
Absolute stereochemistry.

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



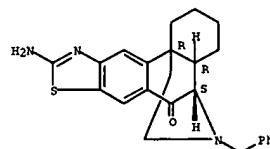
RN 696597-51-0 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(2-propynyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696597-54-3 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(phenylmethyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



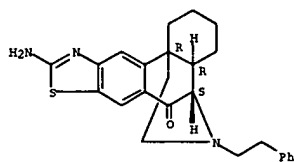
RN 696597-58-7 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-1,2,3,4,4a,5-hexahydro-14-(2-phenylethyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



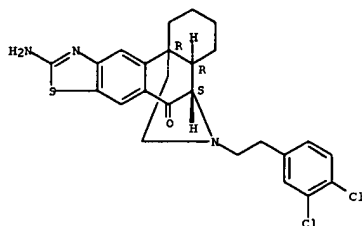
5/09/05

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 696597-62-3 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-[(3,4-dichlorophenyl)ethyl]-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

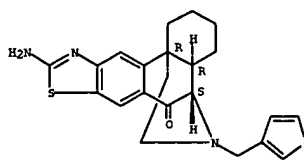
Absolute stereochemistry.



RN 696597-68-9 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-[(3-furanylmethyl)-1,2,3,4,4a,5,6-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

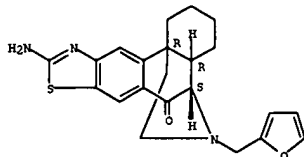
Absolute stereochemistry.

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



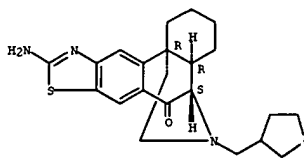
RN 696597-74-7 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-[(2-furanylmethyl)-1,2,3,4,4a,5,6-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 696597-80-5 CAPLUS  
CN 6H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-[(2-furanylmethyl)-1,2,3,4,4a,5,6-hexahydro-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

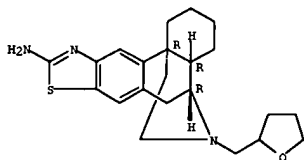


RN 696599-70-9 CAPLUS

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

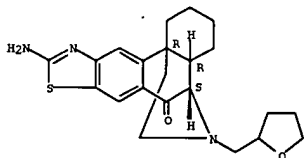
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-[(tetrahydro-2-furanyl)methyl]-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



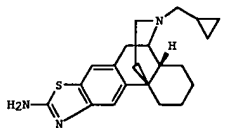
RN 696600-06-3 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-[(tetrahydro-2-furanyl)methyl]-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

GI



AB A series of aminothiazole-derived morphinans, benzomorphan, and morphine were synthesized. Although their affinities were somewhat lower than their phenol prototypes, one compound, designated as ATPM (I), possessed high affinity and selectivity at the  $\kappa$  receptor. Functional assays showed that I was a full  $\kappa$  but partial  $\mu$  agonist; the efficacy at  $\kappa$  was significantly greater than at  $\mu$  receptors. This novel compound may be valuable for the development of long-acting analgesics and drug abuse medication.

IT 682806-53-7P, ATPM 682806-53-9P, ATEM

682806-56-0P, MCL 168

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

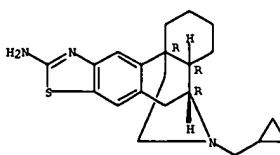
(preparation and opioid receptor binding activity of

2-aminothiazole-derived morphinan, benzomorphan, and morphine opioids)

RN 682806-53-7 CAPLUS

CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine, 14-[(cyclopropylmethyl)-2,3,4,4a,5,6-hexahydro-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



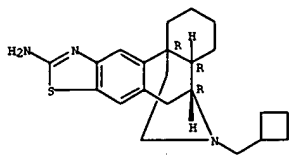
RN 682806-55-9 CAPLUS  
CN 1H-5,11b-(1iminoethano)phenanthro[3,2-d]thiazol-9-amine, 14-[(cyclopropylmethyl)-2,3,4,4a,5,6-hexahydro-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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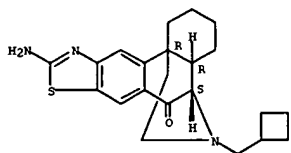
5/09/05

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 682806-56-0 CAPLUS  
CN 6H-5,11b-(1minoethano)phenanthro[3,2-d]thiazol-6-one, 9-amino-14-(cyclobutylmethyl)-, (4aR,5S,11bR)- (9CI) (CA INDEX NAME)

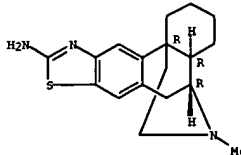
Absolute stereochemistry.



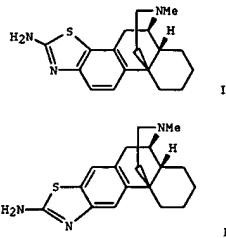
IT 609809-84-9, MCL 186  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation and opioid receptor binding activity of 2-aminothiazole-derived morphinan, benzomorphan, and morphine opioids)  
RN 609809-84-9 CAPLUS  
CN 1H-5,11b-(1minoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-methyl-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



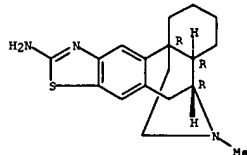
L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
GI



AB Two aminothiazole derived morphinans I and II were prepared for the ongoing opioid ligands study. The synthesis was initiated from levorphanol, which was first triflated, and then subjected to Pd-catalyzed reduction followed by nitration. The resulting two nitrated isomers were characterized by analogy to known compds. The formation of the aminothiazole ring occurred highly selectively to yield only one product from each of the anilines.

IT 609809-84-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of aminothiazole derived morphinans)  
RN 609809-84-9 CAPLUS  
CN 1H-5,11b-(1minoethano)phenanthro[3,2-d]thiazol-9-amine, 2,3,4,4a,5,6-hexahydro-14-methyl-, (4aR,5R,11bR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



10716100

5/09/05

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.32	174.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.19

FILE 'REGISTRY' ENTERED AT 17:44:11 ON 09 MAY 2005  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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provided by InfoChem.

STRUCTURE FILE UPDATES: 8 MAY 2005 HIGHEST RN 850006-33-6  
DICTIONARY FILE UPDATES: 8 MAY 2005 HIGHEST RN 850006-33-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Crossover limits have been increased. See HELP CROSSOVER for details.

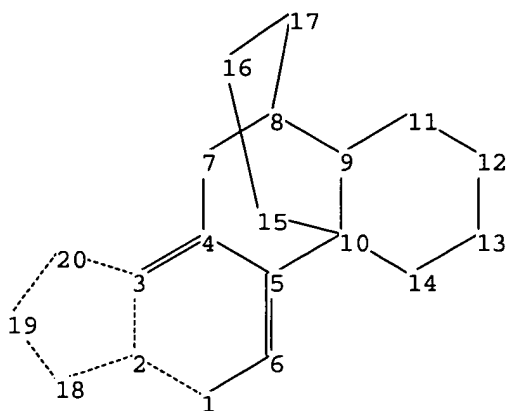
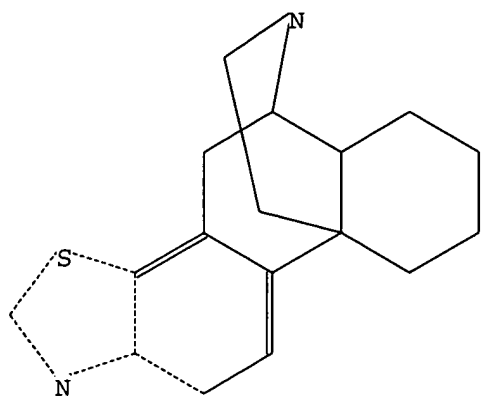
Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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Uploading C:\Program Files\Stnexp\Queries\10716100-2.str

10716100

5/09/05



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10-14 10-15 11-12 12-13 13-14 15-16 16-17 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 2-18 3-4 3-20 4-5 4-7 5-6 5-10 7-8 8-9 8-17 9-10 9-11
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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
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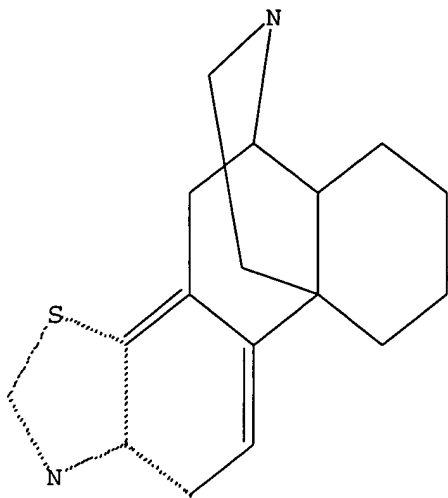
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=> d 15

L5 HAS NO ANSWERS

L5                STR

5/09/05



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 56 TO 504  
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s 15 ful

FULL SEARCH INITIATED 17:44:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 261 TO ITERATE

100.0% PROCESSED 261 ITERATIONS 18 ANSWERS  
SEARCH TIME: 00.00.01

L7 18 SEA SSS FUL L5

=> d his

(FILE 'HOME' ENTERED AT 17:40:59 ON 09 MAY 2005)

FILE 'REGISTRY' ENTERED AT 17:41:07 ON 09 MAY 2005

L1 STRUCTURE UPLOADED  
L2 2 S L1  
L3 36 S L1 FUL

10716100

5/09/05

FILE 'CAPLUS' ENTERED AT 17:41:36 ON 09 MAY 2005

L4 3 S L3

FILE 'REGISTRY' ENTERED AT 17:44:11 ON 09 MAY 2005

L5 STRUCTURE UPLOADED

L6 1 S L5

L7 18 S L5 FUL

=> s l7 not l3

L8 18 L7 NOT L3

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.76	336.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

FILE 'CAPLUS' ENTERED AT 17:45:17 ON 09 MAY 2005

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FILE COVERS 1907 - 9 May 2005 VOL 142 ISS 20

FILE LAST UPDATED: 8 May 2005 (20050508/ED)

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L9 3 L7

=> s l9 not l4

L10 0 L9 NOT L4

=> logoff y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	337.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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10716100

5/09/05

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

STN INTERNATIONAL LOGOFF AT 17:46:01 ON 09 MAY 2005

10716100

5/09/05

=> s 12

L3 3 L2

=> d fbib abs fhitr 1-3

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:452994 CAPLUS

DN 141:7330

TI Mixed kappa/mu opioids and uses thereof

IN Neumeyer, John L.; Zhang, Ao

PA The Mclean Hospital Corporation, USA

SO PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DT Patent

LA English

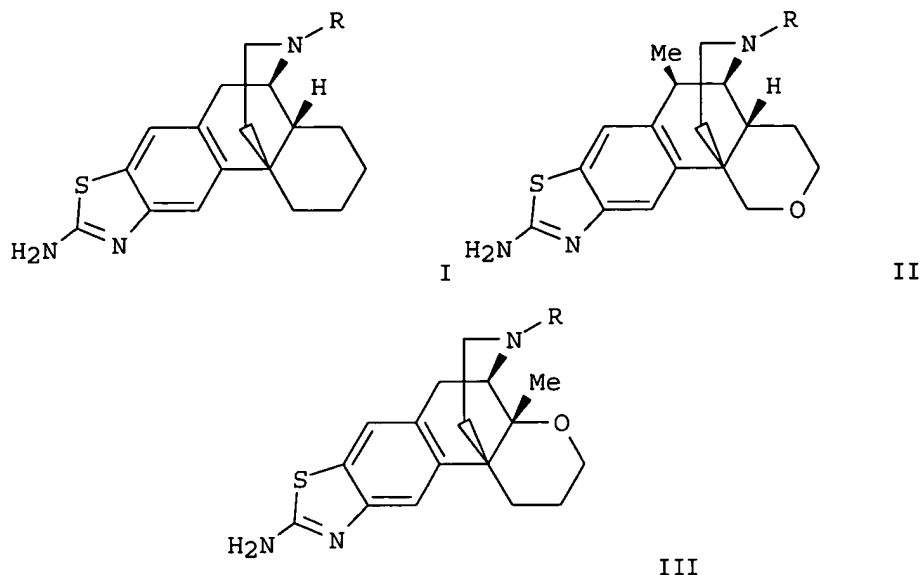
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	WO 2004045562	A3	20040826		
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	RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
				US 2002-427109P	P 20021118
				US 2003-461157P	P 20030408
	US 2004259901	A1	20041223	US 2003-716100	20031118
				US 2002-427109P	P 20021118
				US 2003-461157P	P 20030408
OS	MARPAT 141:7330				
GI					

10716100



5/09/05



AB Various types (i.e I, II, and III (R = H, C1-7 alkyl, C2-7 alkenyl, C2-7 alkynyl, C2-6 heterocyclyl, C6-12 aryl, C7-14 alkaryl, C3-10 alkheterocyclyl, and C1-7 heteroalkyl)) of kappa and mu opioids were prepared for the treatment of pain or a dopamine dysregulation disease, such as schizophrenia, attention deficit hyperactivity disorder (ADHD), attention deficit hyperactivity disorder (ADD), Parkinson's disease, hyperprolactinemia, depression, and addiction. Thus, levorphanol was treated with N-Ph bis(trifluoromethanesulfonimide) and triethylamine to yield the triflate which was reduced using Pd/C (10%) and ammonium formate to give N-Me morphinan. N-Me morphinan was nitrated using HNO<sub>3</sub>/H<sub>2</sub>SO<sub>4</sub> in nitromethanol to give 2-nitro-N-methylmorphinan which was reduced to the amine using Pd/C (10%) and ammonium formate in methanol. Treatment of them amine with potassium thiocyanate and bromine in acetic acid gave the aminothiazole I (R = Me) which has a K<sub>i</sub> of 130 nM for the  $\mu$  receptor and a K<sub>i</sub> of 29 nM for the kappa opioid receptor.

IT **609809-83-8P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of opioid receptor binders for the treatment of pain or dopamine dysregulation diseases)

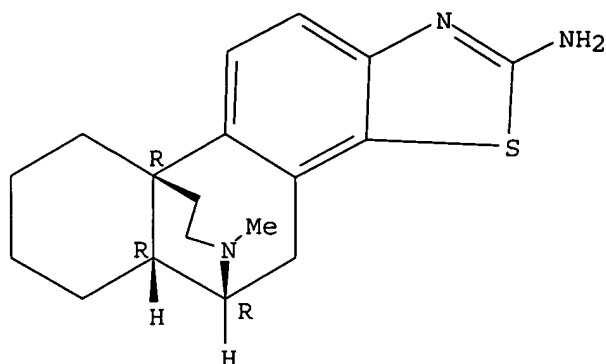
RN 609809-83-8 CAPLUS

CN 4H-5,9a-(Iminoethano)phenanthro[2,1-d]thiazol-2-amine, .  
5,5a,6,7,8,9-hexahydro-14-methyl-, (5R,5aR,9aR) - (9CI) (CA INDEX NAME)

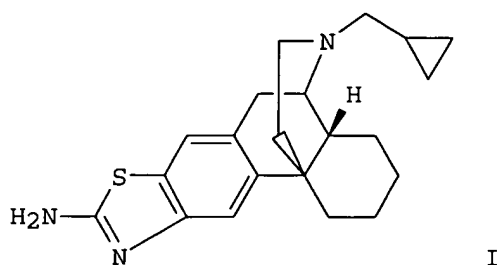
Absolute stereochemistry.

10716100

5/09/05



L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:194846 CAPLUS  
DN 140:357527  
TI 2-Aminothiazole-Derived Opioids. Bioisosteric Replacement of Phenols  
AU Zhang, Ao; Xiong, Wennan; Hilbert, James E.; DeVita, Emily K.; Bidlack,  
Jean M.; Neumeyer, John L.  
CS Alcohol and Drug Abuse Research Center, McLean Hospital, Belmont, MA,  
02478, USA  
SO Journal of Medicinal Chemistry (2004), 47(8), 1886-1888  
CODEN: JMCMAR; ISSN: 0022-2623  
PB American Chemical Society  
DT Journal  
LA English  
GI



AB A series of aminothiazole-derived morphinans, benzomorphans, and morphine were synthesized. Although their affinities were somewhat lower than their phenol prototypes, one compound, designated as ATPM (I), possessed high affinity and selectivity at the  $\kappa$  receptor. Functional assays showed that I was a full  $\kappa$  but partial  $\mu$  agonist; the efficacy at  $\kappa$  was significantly greater than at  $\mu$  receptors. This novel compound may be valuable for the development of long-acting analgesics and drug abuse medication.

IT **609809-83-8**, MCL 187  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation and opioid receptor binding activity of 2-aminothiazole-derived morphinan, benzomorphane, and morphine opioids)

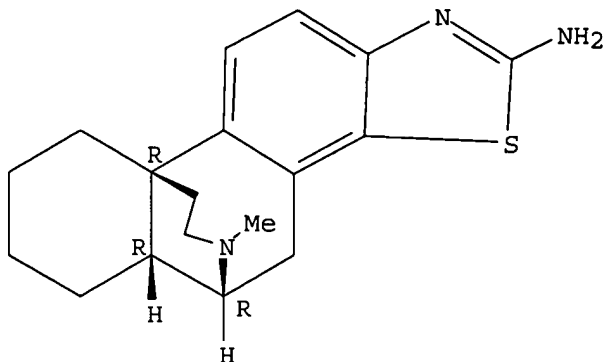
RN 609809-83-8 CAPLUS

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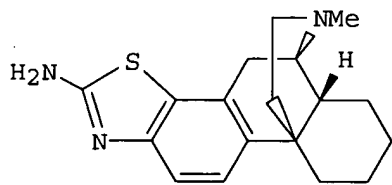
CN 4H-5,9a-(Iminoethano)phenanthro[2,1-d]thiazol-2-amine,  
5,5a,6,7,8,9-hexahydro-14-methyl-, (5R,5aR,9aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

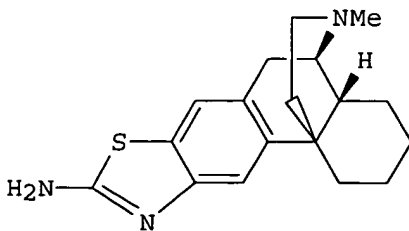


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 2003:597581 CAPLUS  
DN 139:292378  
TI Synthesis of aminothiazole derived morphinans  
AU Zhang, Ao; van Vliet, Sander; Neumeyer, John L.  
CS Alcohol and Drug Abuse Research Center, McLean Hospital, Harvard Medical  
School, Belmont, MA, 02478, USA  
SO Tetrahedron Letters (2003), 44(34), 6459-6462  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier Science B.V.  
DT Journal  
LA English  
OS CASREACT 139:292378  
GI



I



II

10716100

5/09/05

AB Two aminothiazole derived morphinans I and II were prepared for the ongoing opioid ligands study. The synthesis was initiated from levorphanol, which was first triflated, and then subjected to Pd-catalyzed reduction followed by nitration. The resulting two nitrated isomers were characterized by analogy to known compds. The formation of the aminothiazole ring occurred highly selectively to yield only one product from each of the anilines.

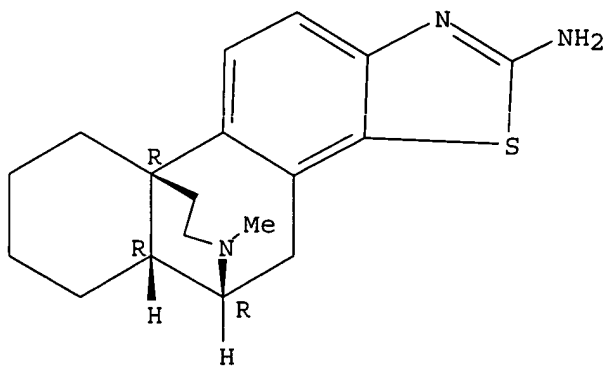
IT **609809-83-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of aminothiazole derived morphinans)

RN 609809-83-8 CAPLUS

CN 4H-5,9a-(Iminoethano)phenanthro[2,1-d]thiazol-2-amine,  
5,5a,6,7,8,9-hexahydro-14-methyl-, (5R,5aR,9aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT